How to simulate the quasi-stationary state

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(February 2, 2008)

Abstract

For a large class of processes with an absorbing state, statistical properties of the surviving sample attain time-independent values in the *quasi-stationary* (QS) regime. We propose a practical simulation method for studying quasi-stationary properties, based on the equation of motion governing the QS distribution. The method is tested in applications to the contact process. At the critical point, our method is about an order of magnitude more efficient than conventional simulation.

PACS: 05.10.-a, 02.50.Ga, 05.40.-a, 05.70.Ln

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Stochastic processes with an absorbing state arise frequently in statistical physics [1,2], epidemiology [3], and related fields. In autocatalytic processes (in lasers, chemical reactions, or surface catalysis, for example), and population models, a population of $n \geq 0$ individuals goes extinct when the absorbing state, $n = 0$, is reached. Phase transitions to an absorbing state in spatially extended systems, exemplified by the contact process [4,5], are currently of great interest in connection with self-organized criticality [6], the transition to turbulence [7], and issues of universality in nonequilibrium critical phenomena [8–10]. Such models are frequently studied using deterministic mean-field equations, Monte Carlo simulation, and renormalization group analyses.

It is desirable to develop additional methods for studying processes with absorbing states. In this work we study models that admit an active (nonabsorbing) stationary state in the infinite-size limit, but which always, for a finite system size, end up in the absorbing state. The *quasi-stationary* (QS) distribution for such a system provides a wealth of information about its behavior. (In fact, simulations of "stationary" properties of lattice models with an absorbing state actually study the quasi-stationary regime, given that the only true stationary state for a finite system is the absorbing one.)

In particular, it would be valuable to have a simulation method that yields quasi-stationary properties directly. Currently available methods involve a somewhat complicated procedure for determining QS properties: a large sample of independent realizations are performed, and the mean $\phi(t)$ of some property (for example the order parameter) is evaluated over the surviving realizations at time t. At short times times $\phi(t)$ exhibits a transient as it relaxes toward the QS regime; at long times it fluctuates wildly as the surviving sample decays. Normally one is able to identify an intermediate regime free of transients and with limited fluctuations, which can be used to estimate the QS value of ϕ. This method requires careful scrutiny of the data and is not always free of ambiguity [11].

A number of strategies have been devised to circumvent the difficulties associated with simulating models exhibiting absorbing states. One involves replacing the absorbing state with a *reflecting* boundary in configuration space [12]. In another approach the activity is fixed at a nonzero value, in a "constant coverage" simulation [13] or a "conserved" version of the model [14]. If one includes a weak external source of activity, h, the zero-activity state is no longer absorbing, but it is possible to obtain information on critical behavior by analyzing scaling properties as $h \to 0$ [11]. A further possibility is to clone surviving realizations of the process, enriching the sample to compensate for attrition as the survival probability decays [15]. While all of these approaches are useful, none affords direct, unbiased sampling of the QS state of the original process.

For models without spatial structure, such as uniformly distributed populations or well stirred chemical reactors, the full QS distribution can be found from the master equation, via recurrence relations or an iterative scheme [16,17]. In models

with spatial structure, typified by nearest-neighbor interactions on a lattice, mean-field like approximations to the QS distribution have been derived, but descriptions in terms of one or a few random variables cannot capture critical fluctuations. The simulation method developed here does not suffer from this limitation. It provides a sampling of the QS probability distribution just as conventional Monte Carlo simulation does for the equilibrium distribution.

We begin reviewing the definition of the quasi-stationary distribution. Consider a continuous-time Markov process X_t taking values $n = 0, 1, 2, ..., S$, with the state $n = 0$ absorbing. We use $p_n(t)$ to denote the probability that $X_t = n$, given some initial state X_0. The survival probability $P_s(t) = \sum_{n\geq 1} p_n(t)$ is the probability that the process has not become trapped in the absorbing state up to time t. We suppose that as $t \to \infty$ the p_n, normalized by the survival probability $P_s(t)$, attain a time-independent form. The quasi-stationary distribution $\overline{p}_n$ is then defined via

$$\overline{p}_n = \lim_{t\to\infty} \frac{p_n(t)}{P_s(t)}, \quad (n \geq 1), \tag{1}$$

with $\overline{p}_0 \equiv 0$. The QS distribution is normalized so:

$$\sum_{n\geq 1} \overline{p}_n = 1. \tag{2}$$

We now discuss the theoretical basis for our simulation method. The QS distribution is the stationary solution to the following equation of motion [16] (for $n > 0$)

$$\frac{dq_n}{dt} = -w_n q_n + r_n + r_0 q_n \ , \tag{3}$$

where $w_n = \sum_m w_{m,n}$ is the total rate of transitions out of state n, and $r_n = \sum_m w_{n,m} q_m$ is the flux of probability into this state. To see this, consider the master equation (Eq. (3) without the final term) in the QS regime. Substituting $q_n(t) = P_s(t)\overline{p}_n$, and noting that in the QS regime $dP_s/dt = -\overline{r}_0 = -P_s \sum_m w_{0,m}\overline{p}_m$, we see that the r.h.s. of Eq. (3) is identically zero if $q_n = \overline{p}_n$ for $n \geq 1$. The final term in Eq. (3) represents a redistribution of the probability r_0 (transfered to the absorbing state in the original master equation), to the nonabsorbing subspace. Each nonabsorbing state receives a share equal to its probability.

Although Eq. (3) is not a master equation (it is nonlinear in the probabilities q_n), it does suggest a simulation scheme for sampling the QS distribution. In a Monte Carlo simulation one generates a set of realizations of a stochastic process. In what follows we call a simulation of the original process X_t (possessing an absorbing state) a *conventional* simulation. Our goal is to define a related process, X_t^*, whose *stationary* probability distribution is the *quasi-stationary* distribution of X_t. (Note

that in order to have a nontrivial stationary distribution, X_t^* cannot possess an absorbing state.) The probability distribution of X_t^* is governed by Eq. (3), which implies that for $n > 0$ (i.e., away from the absorbing state), the evolution of X_t^* is identical to that of X_t. (Since Eq. (3) holds for $n > 0$, the process X_t^* must begin in a non-absorbing state.) When X_t enters the absorbing state, however, X_t^* instead jumps to a nonabsorbing one, and then resumes its "usual" evolution (with the same transition probabilities as X_t), until such time as another visit to the absorbing state is imminent.

A subtle aspect of Eq. (3) is that the distribution q_n is used to determine the value of X_t^* when X_t visits the absorbing state. Although one has no prior knowledge of q_n (or its long-time limit, the QS distribution $\overline{p}_n$), one can, in a simulation, use the history X_s^* $(0 < s \leq t)$ up to time t, to *estimate* the q_n. This is done by saving (and periodically updating) a sample $n_1, n_2, ..., n_M$ of the states visited. (If the state space is characterized by a small set of variables, one may instead accumulate a histogram $H(n)$ giving the time spent in state n.) As the evolution progresses, X_s^* will visit states according to the QS distribution. We therefore update the sample $\{n_1, n_2, ..., n_M\}$ by periodically replacing one of these configurations with the current one. In this way the distribution for the process X_t^* (and the sample drawn from it), will converge to the QS distribution (i.e., the stationary solution of Eq. (3)) at long times. Summarizing, the simulation process X_t^* has the same dynamics as X_t, except that when a transition to the absorbing state is imminent, X_t^* is placed in a nonabsorbing state, selected at random from a sample over the history of the realization. In effect, the nonlinear term in Eq. (3) is represented as a *memory* in the simulation.

To explain how our method works in practice, we detail its application to the *contact process* (CP) [4,5,8]. In the CP, each site i of a lattice is either occupied $(\sigma_i(t) = 1)$, or vacant $(\sigma_i(t) = 0)$. Transitions from $\sigma_i = 1$ to $\sigma_i = 0$ occur at a rate of unity, independent of the neighboring sites. The reverse transition can only occur if at least one neighbor is occupied: the transition from $\sigma_i = 0$ to $\sigma_i = 1$ occurs at rate λr, where r is the fraction of nearest neighbors of site i that are occupied; thus the state $\sigma_i = 0$ for all i is absorbing. (λ is a control parameter governing the rate of spread of activity.) The order parameter ρ is the fraction of occupied sites.

To begin we study the contact process on a *complete graph* (CPCG), in which the rate for a vacant site to turn occupied is λ times the fraction of *all* sites that are occupied, rather than the fraction of nearest neighbors. Since each site interacts equally with all others, all pairs of sites are neighbors, defining a complete graph. (The critical value in this case is $\lambda_c = 1$; the stationary value of ρ is zero for $\lambda < \lambda_c$.) The state of the process is specified by a single variable n: the number of occupied sites. This is a one-step process with nonzero transition rates

$$W_{n-1,n} = n \tag{4}$$

$$W_{n+1,n} = \lambda \frac{n}{L}(L - n) \tag{5}$$

on a graph of L sites. In Ref. [16] the exact QS distribution for the CPCG is obtained via a set of recurrence relations.

We simulate the quasi-stationary state of the CPCG by realizing the process corresponding to the transition rates of Eqs. (4) and (5) and maintaining a list of $M = 10^4$ states. Each time a (nonabsorbing) state is visited, we update the list with probability $\gamma\Delta t$ where $\Delta t = 1/w_n$ is the mean duration of this state. Whenever a transition to the absorbing state ($n = 0$) is generated, we instead select a state from the list. The results for a system of 100 sites, using $\gamma = 0.5$, are shown in Fig. 1, illustrating excellent agreement with the exact QS distribution obtained in Ref. [16]. The simulation result is in good agreement with the exact result even for $\lambda = 0.1$, deep in the subcritical regime, in which the lifetime of the original process is very short.

Next we turn to the one-dimensional contact process (i.e, the model defined above on a ring of L sites). Although no exact results are available, the model has been studied intensively via series expansion and Monte Carlo simulation. In the QS simulations we use a list size $M = 2 \times 10^3$ - 10^4, depending on the lattice size. The process is simulated in runs of 10^8 or more time steps. As is usual, annihilation events are chosen with probability $1/(1+\lambda)$ and creation with probability $\lambda/(1+\lambda)$. A site is chosen from a list of currently occupied sites, and, in the case of annihilation, is vacated, while, for creation events, a nearest-neighbor site is selected at random and, if it is currently vacant, it becomes occupied. The time increment associated with each event is $\Delta t = 1/N_{occ}$, where N_{occ} is the number of occupied sites just prior to the attempted transition [8].

In the initial phase of the evolution, the list of saved configurations is augmented whenever the time t increases by one, until a list of M configurations is accumulated. From then on, we update the list (replacing a randomly selected entry with the current configuration), with a certain probability p_{rep}, whenever t advances by one unit. A given configuration therefore remains on the list for a mean time of M/p_{rep}. (Values of p_{rep} in the range $10^{-3} - 10^{-2}$ are used; the results appear to be insensitive to the precise choice.)

Fig. 2 shows that our method reproduces the order parameter ρ obtained via conventional simulations. In Fig. 3 the QS and conventional results for the moment ratio $m = \langle\rho^2\rangle/\langle\rho\rangle^2$ are compared. As discussed in Ref. [16], the *lifetime* of the QS state is given by $\tau = 1/\overline{p}_1$. The lifetime obtained in QS simulations compares well with the lifetime obtained via conventional simulation (using $P_s \sim \exp(-t/\tau)$), as shown in Fig. 4. Detailed comparison shows that there is no significant difference between the QS and conventional simulation results. For $\lambda < 3$, conventional simulations are subject to relatively large uncertainties, since almost all realizations become trapped in the absorbing state before the quasi-stationary regime is attained. At the critical point, quasi-stationary simulations require about an order of magnitude less cpu time than conventional simulations, to achieve results of the same precision. (Below λ_c the savings is even greater; well above λ_c the two methods

are equally efficient, since visits to the absorbing state are extremely rare.)

As a further application of our method we study the critical CP ($\lambda_c = 3.297848$) on rings of $80, 160, ..., 1280$ sites. We perform between 5 and 30 realizations, each extending to 5×10^8 time steps. Results from the first 10^7 time steps (2×10^7 for $L = 1280$) are discarded from the averages; convergence to the QS state occurs on a considerably shorter time scale. Varying the list size M and the replacement probability p_{rep}, we obtain results consistent with conventional simulations for $M = 1000$ or greater, and $p_{rep} \leq 10^{-2}$. Smaller list sizes and/or larger values of p_{rep} yield results slightly, but significantly, different from previous studies. On the other hand, there seems to be little point in using a list size much greater than the number of reinitializations. In practice the best approach is to use $M = 10^3$ or more, and to perform simulations with several values of p_{rep}, to verify that the results show no significant dependence on this parameter.

Our results permit us to refine the estimate for the moment ratio $m = \langle\rho^2\rangle/\langle\rho\rangle^2$ (ρ denotes the fraction of occupied sites). This quantity is analogous to Binder's reduced fourth cumulant [18] at an equilibrium critical point: the curves $m(\lambda, L)$ for various L cross near λ_c (the crossings approach λ_c as L increases), so that m assumes a universal value m_c at the critical point. In Ref. [19] the estimate $m_c = 1.1736(2)$ for the critical one-dimensional CP was obtained from simulations of systems of up to 320 sites. Using the present method we reproduce and refine the results of [19]. Based on our data for $L \leq 640$ we estimate $m_c = 1.17370(2)$.

At the critical point, the order parameter is expected to decay as a power law, $\rho \sim L^{-\beta\nu_\perp}$. The QS simulation data (for L = 80 - 1280) follow a power law with $\beta\nu_\perp = 0.2525(5)$, compared with the literature value of 0.2521. The lifetime $\tau \sim L^{\nu_{||}/\nu_\perp}$ at the critical point; our simulation results yield $\nu_{||}/\nu_\perp = 1.576(2)$ while the standard value is 1.5807. We find that including a correction to scaling scaling term of the form $\tau \sim L^{\nu_{||}/\nu_\perp}(1 - bL^{-\phi})$ yields a substantially better fit (the sum of the squares of the errors is reduced by a factor of 2) if we use $\phi = 0.2$. The best-fit parameters are $b = 0.069$ and $\nu_{||}/\nu_\perp = 1.581(2)$. (Precise determination of this correction to scaling term will require high precision data for a larger set of system sizes, a task we defer to future work.) Summarizing, the QS simulation method yields results fully consistent with conventional simulation, and with established scaling properties, when applied to the contact process on a ring.

It is interesting to compare the QS distribution with that obtained using a reflecting boundary at $n = 0$, as was used in [12]. In the case of the CP on a complete graph the stationary distribution with a reflecting boundary (RB) is given in [16], where it is called the "pseudo-stationary" distribution. We find that for large systems, in the active phase (λ well above λ_c) the RB and QS distributions are essentially the same, but that nearer (and below) the transition the RB distribution yields a much higher probability for states near $n = 1$ than does the QS. The reflecting boundary is equivalent to a modified process X_t^* which, when a visit to the absorbing state is imminent, is always reset to the previous configuration. Since the latter is but one

step removed from the absorbing state, the buildup of probability in the vicinity is not surprising. In general, we should expect the QS and RB distributions to be in good accord when the lifetime of the process is reasonably long, since this implies a small QS probability in the vicinity of the absorbing state.

In summary, we have devised and tested a simulation method for quasi-stationary properties of models with an absorbing state. The method is easy to implement, and yields reliable results in a fraction of the time required for conventional simulations in the critical regime, of prime interest in the context of scaling and universality. It also opens the possibility of investigating QS properties in the subcritical regime, which is essentially inaccessible to conventional simulations. We expect the method to be applicable to many problems currently under investigation, such as branching-annihilating random walks, conserved sandpiles, and stochastic population models.

Acknowledgment

This work was supported by CNPq and FAPEMIG, Brazil.

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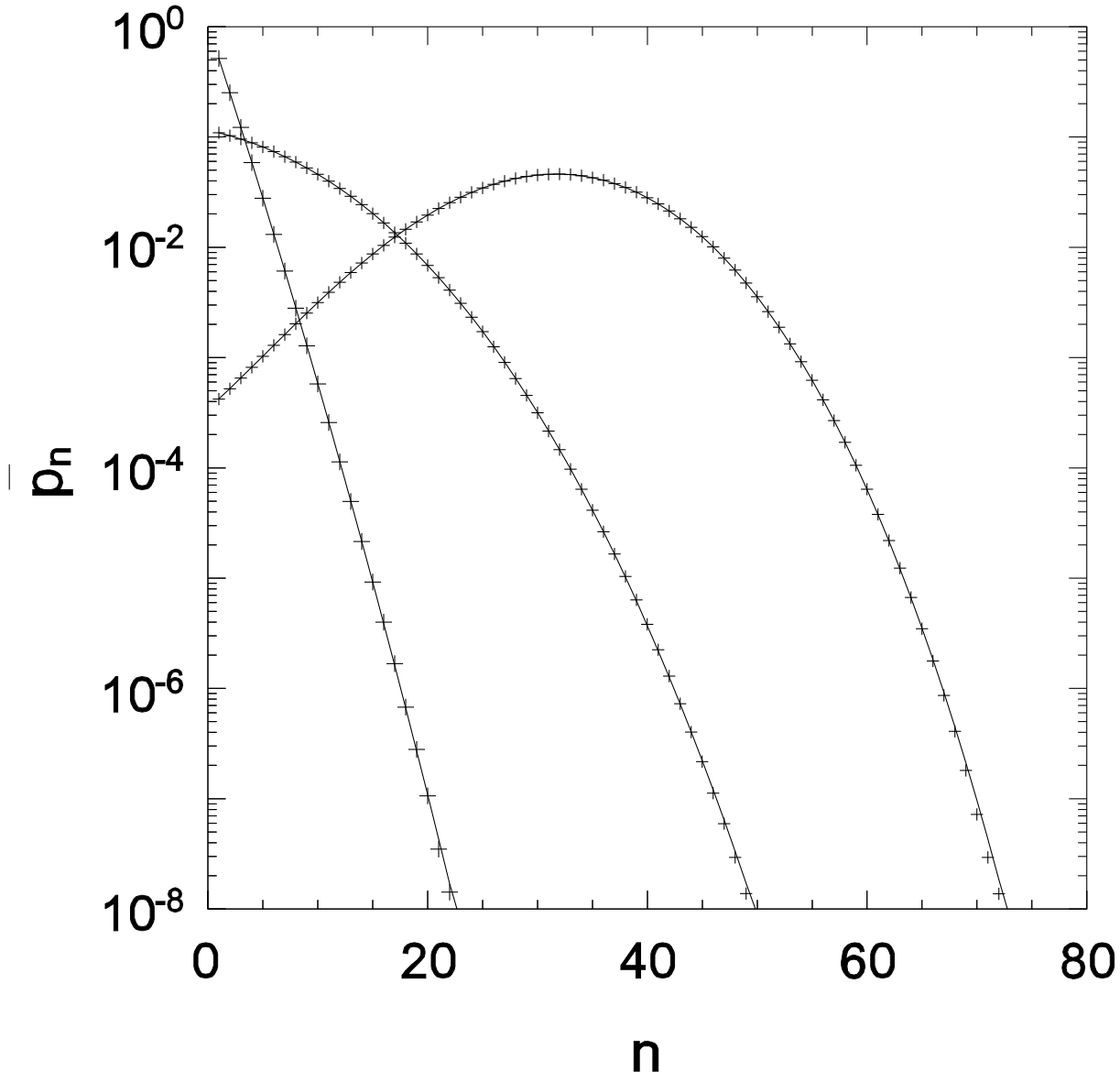
FIGURE CAPTIONS

FIG. 1. QS distributions via recurrence relations (solid lines) and QS simulation (symbols) for the CP on a complete graph of 100 sites. $\lambda = 0.5$, 1.0 and 1.5 (left to right).

FIG. 2.Quasi-stationary density ρ in the one-dimensional CP. Open symbols: QS simulation, $L = 20$; filled symbols: QS simulation, $L = 200$. Solid lines represent results of conventional simulations.

FIG. 3. Quasi-stationary moment ratio M in the one-dimensional CP. Symbols as in Fig. 2.

FIG. 4. Quasi-stationary lifetime τ in the one-dimensional CP. Symbols as in Fig. 2.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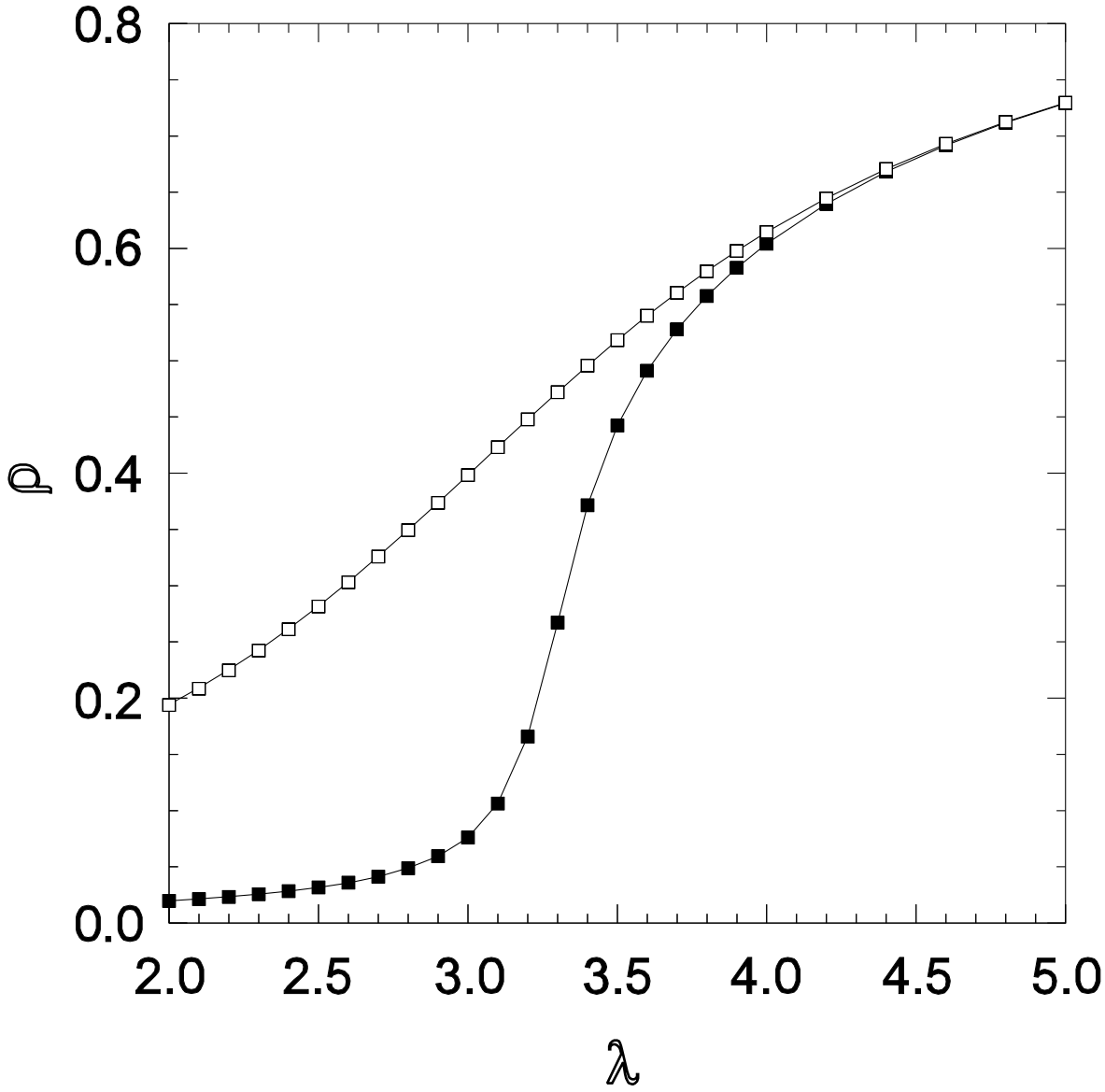
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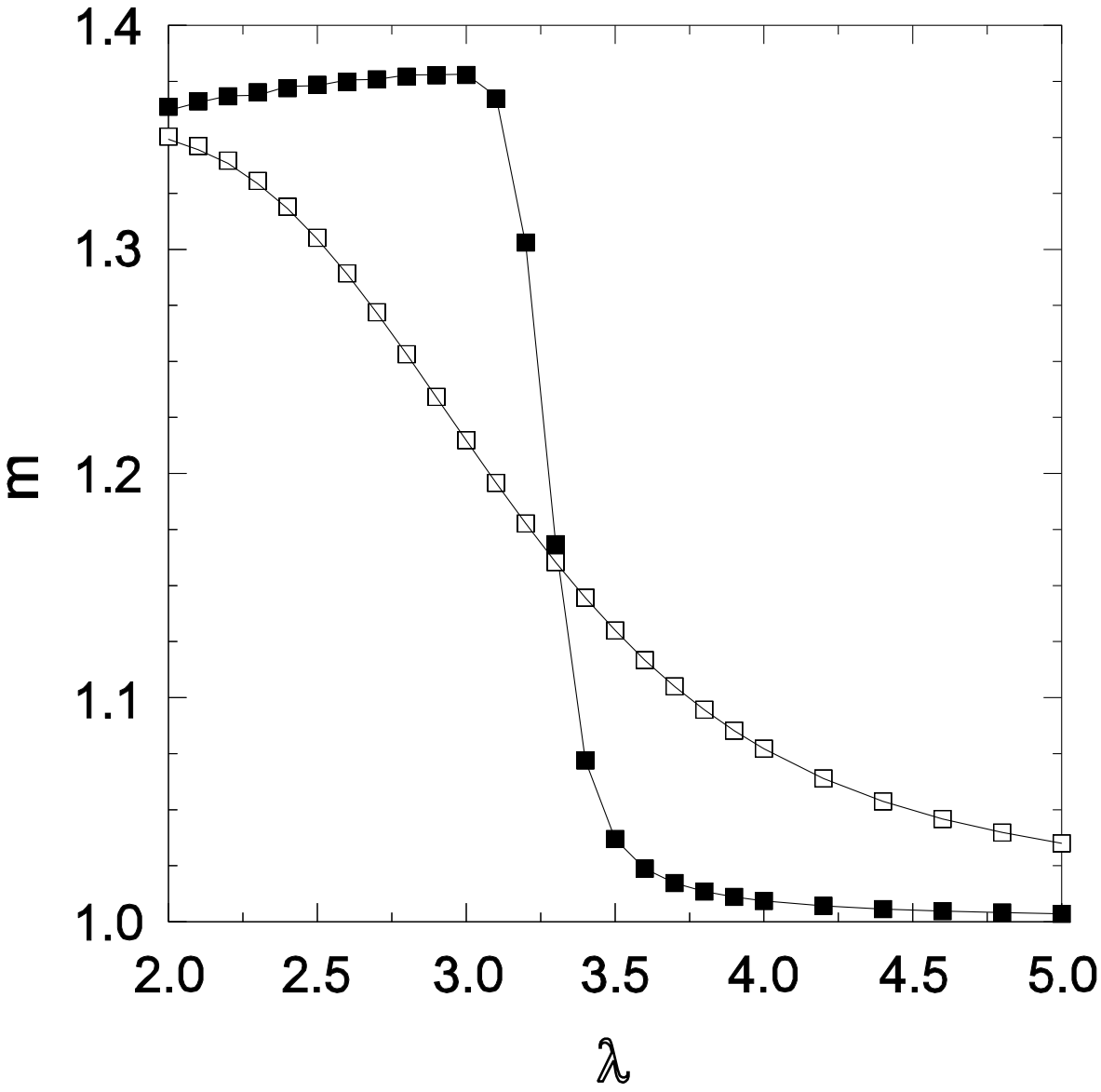
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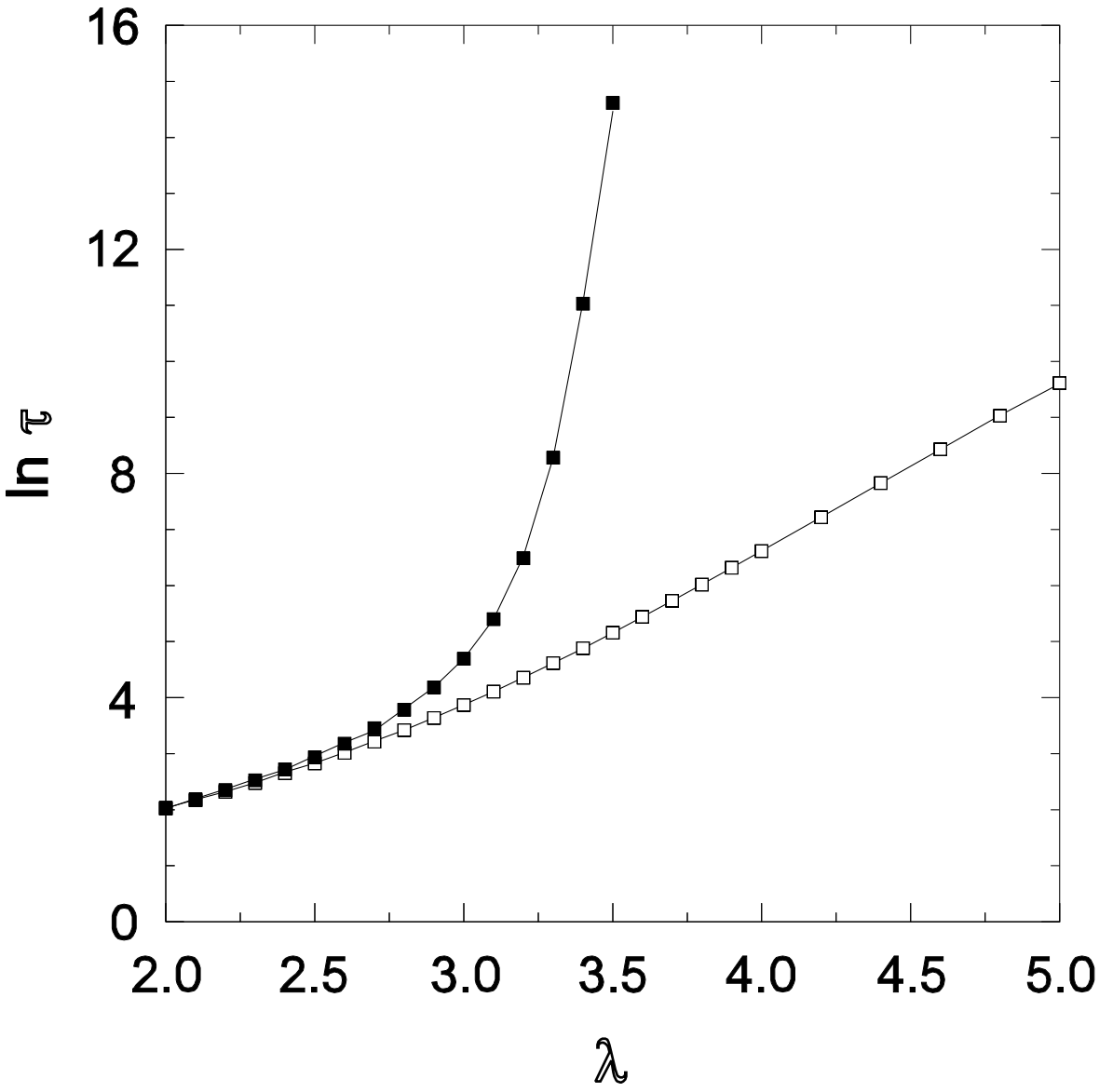
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